

Far-reaching statistical consequences of the zero-point energy for the harmonic oscillator

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Abstract

In a recent thermodynamic analysis of the harmonic oscillator and using an interpolation procedure, Boyer has shown that the existence of a zero-point energy leads to the Planck spectrum. Here we avoid the interpolation by adding a statistical argument to arrive at Planck's law as an inescapable result of the presence of the zero-point energy. No explicit quantum argument is introduced along the derivations. We disclose the connection of our results with the original analysis of Planck and Einstein, which led to the notion of the quantized radiation field. We then inquire into the discrete or continuous behaviour of the energy and pinpoint the discontinuities. Finally, to open the door to the description of the zero-point fluctuations, we briefly discuss the statistical (in contrast to the purely thermodynamic) description of the oscillator, which accounts for both thermal and temperature-independent contributions to the energy dispersion.

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I. INTRODUCTION

In a recent paper^[1] Boyer studies anew the thermodynamics of the harmonic oscillator. By an elementary analysis based on the invariance of the action under a quasistatic change of the frequency, Boyer first reproduces Wien's displacement law (Eq. (2) below). He then introduces an important departure from usual treatments, by allowing for a temperature-independent energy different from zero (the so-called zero-point energy) in solving for the thermodynamic potential at low temperatures. This constitutes an extension of the classical treatment that accords, however, with quantum knowledge. The most immediate evidence of it is that it implies a mean energy proportional to the oscillator's frequency at low temperatures, a result that violates the equipartition principle but agrees with quantum theory.

To derive the Planck equilibrium law from the thermodynamic relations, Boyer makes the smoothest possible interpolation between energy equipartition at high temperatures and zero-point energy at low temperatures. In the present work we show that this interpolation procedure can be avoided by adding a statistical argument to derive the equilibrium spectrum from the sole existence of the zero-point energy. Our approach leads unambiguously to Planck's law and reveals the decisive role of the zero-point energy in defining the quantum behaviour of the system at equilibrium.

As is the case in Boyer's calculation, no explicit quantum argument is introduced along the present derivation. After obtaining our results we review their connection with the original analysis of Planck^[2] and Einstein,^[3] which led to the notion of the quantized radiation field (with no knowledge of the zero-point energy of course), to show explicitly how much simplification and transparency is gained by introducing the idea of the zero-point energy. We further inquire into the discrete or continuous behavior of the energy; the analysis discloses the origin and meaning of the discontinuities.

The thermodynamic analysis carried up to this point is limited, in that the zero-point energy has a sure, nonfluctuating value. Therefore to conclude we briefly discuss the statistical (in contrast to the purely thermodynamic) description, which correctly accounts for both thermal and temperature-independent contributions to the dispersion of the energy and opens the door to the zero-point fluctuations.

II. BASIC RELATIONS

A. Thermodynamics of the harmonic oscillator

In his thermodynamic analysis Boyer shows that the harmonic oscillator can be described by means of a thermodynamic potential $\phi(z)$ (in Boyer's paper the Boltzmann constant, k , is taken as 1 for simplicity)

$$\phi(z) = -\frac{1}{kT}F(\omega, T), \quad z = \frac{\omega}{T}, \quad (1)$$

where $F(\omega, T)$ is the Helmholtz free energy. In particular, the average oscillator energy in thermal equilibrium is given by

$$U(\omega, T) = -\omega k \frac{d\phi(z)}{dz} = -\omega k \phi'(z) = \omega f(\omega/T), \quad (2)$$

where the last equality corresponds to Wien's displacement law. The (thermal) entropy of the oscillator is

$$S(z) = k\phi(z) + \frac{1}{T}U(\omega, T), \quad (3)$$

and for the specific heat at constant volume (and constant ω) Boyer obtains

$$C_V(z) = \left(\frac{\partial U}{\partial T} \right)_{V, \omega} = k z^2 \phi''(z). \quad (4)$$

These results are sufficient for our present purposes. However, before proceeding let us use them to show how it is that the zero-point energy has entered into the picture. In the low-temperature limit ($T \rightarrow 0$), Eq. (2) reads

$$U(\omega, 0) \equiv \mathcal{E}_0 = -\omega k \phi'(\infty) = \text{const} \times \omega. \quad (5)$$

In the usual thermodynamic analysis one *arbitrarily* selects the constant $\phi'(\infty) = 0$. Taking it as different from zero, which is the more general possibility, we see the emergence of a zero-point energy that is proportional to the frequency of the oscillator.^{[5],[6]} This selection, which runs contrary to energy equipartition among the oscillators and hence to 19TH Century classical physics, opens up interesting possibilities that we will explore, following Boyer.

B. Thermodynamic distribution

Our aim is to find the mean energy of the oscillators as a function of the temperature, $\overline{E} = U(T)$. For this purpose we consider a system in equilibrium at temperature T , and

look for a distribution $W(E)$ subject to the demand that the entropy be a maximum. Such entropy is defined through the probability density W by means of the relation

$$S = -k \int W \ln W dE. \quad (6)$$

The maximum entropy formalism^[7] allows us to write the general form of the probability that the energy acquires a value between E and $E + dE$ as

$$W_g(E)dE = \frac{1}{Z_g(\beta)} g(E) e^{-\beta E} dE, \quad (7a)$$

$$Z_g(\beta) = \int g(E) e^{-\beta E} dE. \quad (7b)$$

Here β is the inverse temperature, $\beta = 1/(kT)$; $Z_g(\beta)$ is the partition function and the factor $g(E)$ is the intrinsic probability of the states with energy E . The distribution (7a) is not new; already Einstein considered it in his early works on the investigation of the specific heat of solids.^{[8], [9]}

That this distribution is consistent with the thermodynamics derived by Boyer can be easily seen by mere substitution of (7a) in (6),

$$S = -k \int W_g (-\ln Z_g + \ln g - \beta E) dE = k \ln Z_g - k \overline{\ln g} + U/T. \quad (8)$$

Comparison with Eq. (3) gives for the thermodynamic potential

$$\phi = \ln Z_g - \overline{\ln g}. \quad (9)$$

As shown in Appendix B the term $\overline{\ln g}$ is a numerical constant, so that Eq. (9) leads to

$$\phi' = \frac{d\phi}{dz} = \frac{1}{\omega k} \frac{1}{Z_g} \frac{\partial Z_g}{\partial \beta} = -\frac{1}{\omega k} U, \quad (10)$$

in agreement with Eq. (2).

In standard classical theory all energies are assumed to have equal intrinsic probabilities and thus $g(E) = 1$, which leads to

$$W_{g=1}(E) = \frac{1}{Z_1(\beta)} e^{-\beta E}, \quad Z_1(\beta) = \int_0^\infty e^{-\beta E} dE = \frac{1}{\beta}, \quad \overline{E} = -\frac{1}{Z_1} \frac{dZ_1}{d\beta} = \frac{1}{\beta}, \quad (11)$$

which is contrary to the existence of a zero-point energy. Consequently, in order to allow for a zero-point energy different from zero we must resort to the more general probability density (7a), with $g(E)$ a function to be determined.

III. FUNCTIONAL FORM FOR THE MEAN ENERGY

A. Basic statistical relations

From Eqs. (7) it follows that (from now on the prime indicates derivative with respect to β)

$$\overline{E^r}' = -\frac{Z_g'}{Z_g}\overline{E^r} - \frac{1}{Z} \int_0^\infty E^{r+1} g(E) e^{-\beta E} dE = -\frac{Z_g'}{Z_g}\overline{E^r} - \overline{E^{r+1}}. \quad (12)$$

Since

$$\overline{E} = \frac{1}{Z_g} \int_0^\infty E g(E) e^{-\beta E} dE = -\frac{Z_g'}{Z_g}, \quad (13)$$

Eq. (12) gives the recurrence relation

$$\overline{E^{r+1}} = \overline{E} \overline{E^r} - \overline{E^r}'. \quad (14)$$

Incidentally this result can be extended to any continuous function $G(E)$, to give

$$-\overline{G(E)'} = \overline{EG(E)} - \overline{E} \overline{G(E)}, \quad (15)$$

which shows that $-\overline{G(E)'}$ is given in general by the covariance of $G(E)$ and E .

In particular, for the second moment ($r = 1$ in Eq. (14)) one gets for the energy variance

$$\sigma_E^2 \equiv \overline{E^2} - U^2 = -U'. \quad (16)$$

This equation can be cast as the well known relation^[10]

$$\sigma_E^2 = -U' = kT^2 \left(\frac{\partial U}{\partial T} \right)_{V,\omega} = kT^2 C_V \quad (17)$$

in terms of the heat capacity at constant volume C_V . Since C_V remains finite, the right hand side takes the value 0 at $T = 0$, whence

$$\sigma_E^2(T = 0) = 0, \quad (18)$$

which means that all fluctuations are suppressed at zero temperature. This result refers to *thermal* fluctuations, since the description provided by the distribution W_g is of a thermodynamic nature (W_g was constructed by demanding consistency with the thermodynamic relations only). The existence, description and origin of temperature-independent fluctuations will be discussed below.

B. Establishing the equilibrium spectrum

Our task now is to determine the mean energy $U(\beta)$, using Eq. (16) subject to the condition (18). As follows from (16), it is possible to express σ_E^2 as a function of U by inverting $\overline{E(\beta)} = U$ to express β as a function of the mean energy. Assuming that the resulting expression for $\sigma_E^2(U)$ admits a power series expansion, we write it in the form

$$\sigma_E^2(U) = \sum_{n=0} a_n U^n, \quad (19)$$

where the coefficients a_n can depend only on the fixed parameter ω . Now we demand that the relative dispersion σ_E/U remains finite for all values of U , whence the expression

$$\frac{\sigma_E^2}{U^2} = \frac{a_0}{U^2} + \frac{a_1}{U} + a_2 + a_3 U + a_4 U^2 + \dots \quad (20)$$

must remain finite for every U . In particular, since U (being an increasing function of T) can increase indefinitely, it follows that the coefficients a_n must vanish for $n \geq 3$, whence

$$\sigma_E^2(U) = a_0 + a_1 U + a_2 U^2. \quad (21)$$

Further, if at low temperatures U goes to zero, coefficient a_0 and a_1 must be equal to zero for σ_E/U to remain finite. However, if at low temperatures U does not vanish, the three coefficients can have in principle a nonzero value.

We notice that the dispersion of the energy

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \quad (22)$$

is invariant under the inversion $E \rightarrow -E$. Since this transformation induces the substitution $U \rightarrow -U$, σ_E^2 must be an even function of the variable U , and therefore $a_1 = 0$ in (21),

$$\sigma_E^2(U) = a_0 + a_2 U^2. \quad (23)$$

In Appendix A we demonstrate that $a_1 = 0$ follows directly from Wien's law for $\mathcal{E}_0 > 0$. Combining this with Eq. (16) we obtain

$$\frac{dU}{a_0 + a_2 U^2} = -d\beta, \quad (24)$$

which after integration gives

$$\beta = \begin{cases} \frac{1}{a_2 U} & \text{for } q = 0; \\ \frac{2}{\sqrt{q}} \coth^{-1} \frac{2a_2 U}{\sqrt{q}} & \text{for } q > 0; \end{cases} \quad q \equiv -4a_0 a_2. \quad (25)$$

The case $q < 0$ is excluded for real values of the energy (see equation (27) below). Although the case $q = 0$ can be treated as a limit case of $q \geq 0$, it is more illustrative to deal with the two cases separately. Inverting the functions in (25) we find

$$U(\beta) = \begin{cases} \frac{1}{a_2\beta}, & \text{for } q = 0; \\ \frac{\sqrt{q}}{2a_2} \coth \frac{\sqrt{q}}{2}\beta, & \text{for } q > 0. \end{cases} \quad (26)$$

The behaviour of the mean energy is seen to depend critically on the value of q , a parameter that appears naturally in the expression for the roots of the equation $\sigma_E^2 = 0$,

$$U_{\pm} = \pm \frac{\sqrt{q}}{2a_2}. \quad (27)$$

Since $U(T = 0) = \mathcal{E}_0$, it follows from Eq. (18) that $\sigma_E^2(\mathcal{E}_0) = 0$, so \mathcal{E}_0 is certainly one of the roots U_{\pm} . Further, since the dispersion is an increasing function of the energy ($U(\beta) \geq \mathcal{E}_0$) it follows that $a_2 > 0$, and so \mathcal{E}_0 is given by

$$\mathcal{E}_0 = \frac{\sqrt{q}}{2a_2} = \sqrt{-\frac{a_0}{a_2}} \quad (28)$$

(the other root being unphysical). This relation between q and \mathcal{E}_0 , along with Eq. (26), shows how the functional form of the mean energy is uniquely determined by the zero-point energy. In particular, for a theory with null value for \mathcal{E}_0 we have $q = 0$, $a_0 = 0$ and from (26), $U = (a_2\beta)^{-1}$. Comparison with the classical case compels us to set $a_2 = 1$, whence

$$U = kT. \quad (29)$$

If, however, the theory allows for a zero-point energy $\mathcal{E}_0 \neq 0$, q acquires a value different from 0 as follows from Eq. (28). The latter equation, together with Eq. (26), leads to

$$U(\beta) = \mathcal{E}_0 \coth a_2 \mathcal{E}_0 \beta. \quad (30)$$

Further, by taking the limit $T \rightarrow \infty$ ($\beta \rightarrow 0$) we get

$$U(\beta \rightarrow 0) = \frac{1}{a_2\beta}. \quad (31)$$

The condition that at high temperatures the result (30) coincides with the classical one fixes $a_2 = 1$ as before, whence we finally have

$$U(\beta) = \mathcal{E}_0 \coth \mathcal{E}_0 \beta. \quad (32)$$

This is Planck's law with zero-point energy included, as follows by taking the zero-temperature limit $T \rightarrow 0$ ($\beta \rightarrow \infty$),

$$U(\beta \rightarrow \infty) = \mathcal{E}_0. \quad (33)$$

and recalling from Eq. (5) that $\mathcal{E}_0 = \text{const} \times \omega$.

This establishes Planck's spectral distribution law as a physical result whose ultimate meaning is the existence of a zero-point energy, whereas the equipartition of energy reflects its absence, in full accordance with Boyer's remarks.^[1]

It is important to stress that Planck's law has been obtained without introducing any *explicit* quantum demand. However, the fact that the law that gave birth to quantum theory stems from the existence of a zero-point energy, brings to the fore the crucial importance of this temperature-independent energy for the understanding of quantum mechanics.

IV. PLANCK, EINSTEIN AND THE ZERO-POINT ENERGY

Having fixed the parameter $a_2 = 1$, the value of a_0 follows from Eq. (28)

$$q = 4\mathcal{E}_0^2, \quad a_0 = -\mathcal{E}_0^2. \quad (34)$$

Substitution of these values in Eq. (23) gives for the energy dispersion

$$\sigma_E^2(U) = U^2 - \mathcal{E}_0^2 \quad (U = U_{\text{Planck}}), \quad (35)$$

whereas in the classical case $q = 0$, $\mathcal{E}_0 = 0$ and

$$\sigma_E^2(U) = U^2 \quad (U = U_{\text{equipartition}}). \quad (36)$$

Whilst in the latter case the thermal fluctuations of the oscillator's energy depend on its thermal mean energy, in the quantum case they are expressed in terms of the total mean energy including a temperature-independent contribution, according to Eq. (35). At $T = 0$ however, the thermal fluctuations of the energy vanish in the quantum case just as in the classical case — which means that any fluctuation of the energy at zero temperature must be non-thermal. Below we show that a result similar in form to Eq. (36) holds good in the general case, once all (thermal and non-thermal) fluctuations and energies are taken into account by using a complete statistical description. Since σ_E^2 in Eq. (35) contains *only*

thermal fluctuations, it means that \mathcal{E}_0^2 stands for the fluctuations of the zero-point energy, a result that is verified by Eq. (36).

The above discussion suggests the time-honoured convention of separating the average energy U into a thermal U_T and a temperature-independent \mathcal{E}_0 contribution,

$$U = U_T + \mathcal{E}_0. \quad (37)$$

Substitution in (35) then gives

$$\sigma_E^2 = U_T^2 + 2\mathcal{E}_0 U_T, \quad (38)$$

and since $dU/d\beta = dU_T/d\beta$, it follows using Eq. (16) that

$$-\frac{dU_T}{d\beta} = U_T^2 + 2\mathcal{E}_0 U_T. \quad (39)$$

No wonder that the appropriate solution to this equation for $\mathcal{E}_0 \neq 0$ is the Planck spectrum without the zero-point term,

$$U_T = \frac{2\mathcal{E}_0}{e^{2\mathcal{E}_0\beta} - 1}. \quad (40)$$

At sufficiently low temperatures ($\beta \rightarrow \infty$) this solution takes the form

$$U_T = 2\mathcal{E}_0 e^{-2\mathcal{E}_0\beta}, \quad (41)$$

which is the (approximate) distribution suggested by Wien at the end of the 19TH century.

Equations (38) and (41) were decisive for the initial construction of quantum theory since they led Einstein and Planck to establish the existence of quanta. Let us now briefly discuss the above results and the role played by the then hidden zero-point energy, by paying attention to two fundamental moments in the development of quantum theory.^[11]

A. Planck's analysis...

In his initial studies on the radiation field in equilibrium with matter, Planck^[2] used as point of departure the expression

$$\frac{\partial S}{\partial U} = \frac{1}{T}. \quad (42)$$

In agreement with the then classical views that recognized only a thermal energy, there was no room for a zero-point energy, so that U should be replaced by U_T . In the high-temperature limit the relation (42) led Planck to write (taking $U_T(T \rightarrow \infty) = kT$)

$$\frac{\partial^2 S}{\partial U_T^2} = \frac{\partial}{\partial U_T} \left(\frac{k}{U_T} \right) = -\frac{k}{U_T^2}. \quad (43)$$

However, for his description of the low-temperature behaviour Planck used Wien's law Eq. (41), believed in those days to be an exact description of the properties of the equilibrium field (at the low temperatures tested at the time). He thus wrote (using modern notation, with $\mathcal{E}_0 = \hbar\omega/2$)

$$U_T = 2\mathcal{E}_0 e^{-2\mathcal{E}_0\beta} = 2\mathcal{E}_0 e^{-2\mathcal{E}_0/kT} = 2\mathcal{E}_0 e^{-2(\mathcal{E}_0/k)(\partial S/\partial U_T)}, \quad (44)$$

whence

$$\frac{\partial S}{\partial U_T} = -\frac{k}{2\mathcal{E}_0} \ln \frac{U_T}{2\mathcal{E}_0} \quad (45a)$$

and

$$\frac{\partial^2 S}{\partial U_T^2} = -\frac{k}{2\mathcal{E}_0 U_T}. \quad (45b)$$

As is well known, Planck correctly assumed that the description for arbitrary temperature could be obtained from a direct interpolation of Eqs. (43) and (45b), so he proposed to write

$$\frac{\partial^2 S}{\partial U_T^2} = -\frac{k}{U_T^2 + 2\mathcal{E}_0 U_T}. \quad (46)$$

This leads immediately to Planck's law without zero-point term (Eq. (40)), a result that Planck interpreted afterwards as due to the quantization of the interchanged energy between the material oscillators and the equilibrium radiation field.

B. Einstein's overture...

A few years thereafter, Einstein argued that Eq. (46) was well confirmed by experiment and should therefore be used instead of previous flawed alternatives, though its meaning remained to be clarified. From Eq. (42), which Einstein took as a secure point of departure stemming from thermodynamics,

$$\frac{\partial^2 S}{\partial U_T^2} = \frac{\partial}{\partial U_T} \frac{1}{T} = -\frac{1}{T^2 C_V}, \quad (47)$$

one obtains

$$kT^2 C_V = -k \left(\frac{\partial^2 S}{\partial U_T^2} \right)^{-1}. \quad (48)$$

Combining this with Eqs. (46) and (17) one is led to

$$kT^2 C_V = -\frac{\partial U_T}{\partial \beta} = \sigma_E^2 = U_T^2 + 2\mathcal{E}_0 U_T, \quad (49)$$

which reproduces Eq. (38). Because this expression is at variance with the classical result $\sigma_E^2 = U_T^2$, Einstein took upon himself to decipher its meaning. As is frequently stated, it is here where he brought off his most (according to him, his only) revolutionary step in physics. He interpreted the first term on the right hand side of Eq. (49) as due to the fluctuations of the thermal field (of a given frequency) produced by the interferences among its modes. This interpretation follows from considering the limit of Eq. (49) for high temperatures, for which $U_T \gg \mathcal{E}_0$, and therefore $\sigma_E^2 = U_T^2$, as predicted by Maxwell's equations (without zero-point energy, of course).^[12] Thus Einstein saw in this term a direct manifestation of the undulatory nature of light.

As for the second term in (49) — unexpected from classical thermodynamics — the fact that it leads to the (quantum) theory of Planck induced Einstein to interpret it in terms of light quanta; that is, he saw in the expression $2\mathcal{E}_0 U_T$ the manifestation of a discrete property of the radiation field. According to Planck, the average interchanged energy between the material oscillators and the radiation field is $\Delta U = \hbar\omega\bar{n}$ and the extra fluctuations contribute with a variance $\sigma_{\Delta U}^2 = 2\mathcal{E}_0\Delta U = \hbar^2\omega^2\bar{n}$, as follows from Eq. (49). Einstein argued that the linear character of the variance in \bar{n} suggests a Poisson distribution that describes n independent events, each one interchanging an energy equal to $\hbar\omega$. Thus Einstein interpreted the linear term as a "corpuscular" contribution of the field, each corpuscle being an independent packet of energy $\hbar\omega$ — the photon, in our modern parlance.^[12] This was indeed the birth of the photon theory. It is clear from Eq. (49) that such discrete structure of the field will manifest itself at very low temperatures, where the linear term dominates over the quadratic, undulatory one. However, as stressed by Einstein from 1909 onwards, both terms coexist at all temperatures, and thus both particle and wave properties of the light coexist.^[3]

C. ... and the zero-point energy

At this stage it is interesting to make some comments on Einstein's analysis of Eq. (49). According to Einstein, the first term on the right hand side (U_T^2) is a manifestation of the undulatory nature of the (monochromatic) thermal field, whereas the second one ($2\mathcal{E}_0 U_T$) reflects its quantum aspect. No zero-point energy is considered and a corpuscular property of the radiation field emerges. However, we have seen that the acceptance of a zero-point

energy gives rise to an alternative understanding of Eq. (49). By allowing for a zero-point contribution to the energy, the interference interpretation of the term U_T^2 suggests to understand the term $2\mathcal{E}_0 U_T$ as due to additional interferences between the thermal field and a zero-point field ultimately responsible for the zero-point energy. There is no extra contribution \mathcal{E}_0^2 in Eq. (49) that stands for the interferences among the modes of the zero-point field itself because the present thermodynamic description has no room for the temperature-independent fluctuations of the zero-point energy, as has already been pointed out.

We see that within this restricted approach, no intrinsic discontinuities in the field or in the interchange of energy are needed to derive Planck's law, the existence of a zero-point energy being enough to understand the equilibrium spectrum that follows from Eqs. (46) and (49). This, of course, could not be Planck's or Einstein's interpretation since the zero-point energy was still unknown at that time, and Planck deemed himself forced to introduce the notion of quantization. Anyhow, we have here three different perspectives on the same quantity $U_T^2 + 2\mathcal{E}_0 U_T$.

As said above, Einstein was led for the first time^[13] to his photon theory by the term $2\mathcal{E}_0 U_T$, which he got from Wien's law Eq. (41). This approximate expression already contains the constant \mathcal{E}_0 , through which the seed of the zero-point energy was planted in the results obtained by Planck and Einstein, although due to the circumstances they were unable to interpret them in such terms. Our discussion reinforces the conclusion reached in the previous section about the univocal relation between the zero-point energy and the Planck equilibrium spectrum, bolstering at the same time the need to inquire about the relationship between the zero-point energy and quantization. This we take as our next subject.

V. CONTINUOUS VS DISCRETE

As seen from Eqs. (46) and (49), both Planck and Einstein came up with the binomial $U_T^2 + 2\mathcal{E}_0 U_T$ whose structure was eventually attributed to a discrete, corpuscle-like property of the radiation field. Within the present approach, by contrast, this expression can be interpreted as a direct result of the existence of the zero-point energy, with no apparent need to resort to discontinuities. Our discussion thus suggests that Planck and Einstein were unknowingly using the zero-point energy, concealed by the classical thermodynamic treatment

and accounted for by the quantum description. This is a most inspiring hallmark, which leads us to analyse the apparent contradiction between both approaches: Is quantization necessarily linked to Planck's law, or is it not? Is it merely the result of a point of view, or does it reflect and describe a true, ontological property of nature?

A. The partition function

As follows from Eq. (13), once $U(\beta)$ is known it is possible to determine the partition function $Z_g(\beta)$ by direct integration of

$$U = -\frac{d \ln Z_g(\beta)}{d\beta}. \quad (50)$$

Substituting Eq. (32) gives

$$\int \mathcal{E}_0 \coth \mathcal{E}_0 \beta \, d\beta = -\ln Z_g + \ln C,$$

which leads to

$$Z_g = \frac{C}{\sinh \mathcal{E}_0 \beta}. \quad (51)$$

The value of the constant C can be determined by demanding that in the limit $T \rightarrow \infty$ the classical result $Z_g(\beta \rightarrow 0) = \beta^{-1}$ be recovered. This leads to $C = \mathcal{E}_0$ and

$$Z_g(\beta) = \frac{\mathcal{E}_0}{\sinh \mathcal{E}_0 \beta}. \quad (52)$$

As follows from Eq. (8), the entropy of the system is given by ($z = \omega/T$)

$$S(z) = k\phi(z) + k\beta U(\omega, T) + c = -k \ln (\sinh \mathcal{E}_0 \beta) + k\mathcal{E}_0 \beta \coth \mathcal{E}_0 \beta + k \ln \mathcal{E}_0 - k \overline{\ln g} + c, \quad (53)$$

where the value of the additive constant c is determined by setting $S(T = 0) = 0$,

$$c = -k \ln 2\mathcal{E}_0 + k \overline{\ln g}, \quad (54)$$

and therefore Eq. (53) reduces to

$$S(z) = -k \ln (2 \sinh \mathcal{E}_0 \beta) + k\mathcal{E}_0 \beta \coth \mathcal{E}_0 \beta, \quad (55)$$

which coincides with the result reported in Boyer's paper (with $k = 1$).^[1]

B. The origin of discreteness

Let us now proceed to reveal the discontinuities characteristic of the quantum description, which are hidden under the fully continuous description afforded by the distribution W_g . To this aim we expand Eq. (52) and write^[14]

$$Z_g = 2\mathcal{E}_0 \frac{1}{2 \sinh \mathcal{E}_0 \beta} = 2\mathcal{E}_0 \frac{e^{-\mathcal{E}_0 \beta}}{1 - e^{-2\mathcal{E}_0 \beta}} = 2\mathcal{E}_0 \sum_{n=0}^{\infty} e^{-\mathcal{E}_0 \beta (2n+1)}, \quad (56)$$

or

$$Z_g = 2\mathcal{E}_0 \sum_{n=0}^{\infty} e^{-\beta E_n}, \quad E_n \equiv (2n+1)\mathcal{E}_0. \quad (57)$$

This expression allows us to determine the function $g(E)$ by means of the relation (7b),

$$Z_g(\beta) = \int_0^{\infty} g(E) e^{-\beta E} dE = 2\mathcal{E}_0 \sum_{n=0}^{\infty} e^{-\beta E_n} \equiv 2\mathcal{E}_0 Z, \quad (58a)$$

where we have introduced the dimensionless partition function

$$Z = \sum_{n=0}^{\infty} e^{-\beta E_n} = \frac{1}{2 \sinh \mathcal{E}_0 \beta}. \quad (58b)$$

Thus $g(E)$ can be cast as

$$g(E) = 2\mathcal{E}_0 \sum_{n=0}^{\infty} \delta(E - E_n). \quad (59)$$

Substitution of (58a) and (59) in (7a) results in

$$W_g(E) = \frac{1}{Z} \sum_{n=0}^{\infty} \delta(E - E_n) e^{-\beta E_n}. \quad (60)$$

This distribution gives for the mean value of any function $f(E)$

$$\overline{f(E)} = \int_0^{\infty} W_g(E) f(E) dE = \frac{1}{Z} \sum_{n=0}^{\infty} f(E_n) e^{-\beta E_n} = \sum_{n=0}^{\infty} w_n f(E_n), \quad (61)$$

where we have introduced the weights (relative probabilities)

$$w_n = \frac{e^{-\beta E_n}}{Z} = \frac{e^{-\beta E_n}}{\sum_{n=0}^{\infty} e^{-\beta E_n}}. \quad (62)$$

Eq. (61) shows that the mean value of any function of the continuous variable E weighted with the distribution $W_g(E)$, can equivalently be written as an average weighted with w_n over a set of discrete indices n . Since we are describing a canonical ensemble, the structure of

w_n suggests to identify the quantity E_n with discrete energy levels of the quantum oscillators including of course the zero-point energy, as follows from (57). Thus we can recognize in Eq. (62) the description afforded by the density matrix for the canonical ensemble with weights w_n .^[15]

Even though both averages (those calculated by means of W_g and w_n) are formally equivalent, it must be pointed out that the descriptions afforded by each of these distributions are essentially different, referring to a continuous or a discrete energy, respectively. The expansion in Eq. (61) allows to pass from a description involving an averaging over the in principle continuous variable E to another one involving a summation over discrete *states* n . Since the energy in this new context (E_n) is completely characterized by these states, it becomes natural to interpret the right hand side of (61) as a manifestation of the discrete nature of the energy. The mechanism leading to them, seemingly excluding all other values of the energy, is of course identified with the highly pathological distribution $g(E)$.

These observations show how deeply the introduction of a zero-point energy agrees with the quantum notion introduced by Planck and Einstein, and serves to discover the fundamental role of the zero-point energy in explaining quantization, it being at the root of Eq. (56) and hence of (59).

VI. A QUANTUM STATISTICAL DISTRIBUTION

The analysis just presented leads us to conclude that although E is a continuous variable, its mean values corresponding to the thermodynamic equilibrium states of a canonical ensemble of oscillators are extremely peaked and approximate very closely a discrete spectrum. That is to say, the energies that conform the thermal equilibrium state described by the distribution W_g belong, roughly speaking, to a discrete spectrum. This explains why the mean value $\overline{f(E)}$ — that corresponds to an equilibrium state — involves only the discrete set E_n .

To this, however, we should add that nevertheless the energy fluctuates, and can therefore acquire values from among a continuous spectrum.^[16] As was stated at the beginning of Section IV, the existence of a zero-point energy in the thermodynamic description of the harmonic oscillator demands looking for a more general distribution (instead of W_g) that could account for *all* fluctuations of the energy, including any temperature-independent

contribution. That such distribution must exist follows from the previous results showing that the zero-point energy approach (starting from a continuous energy distribution) led to a result that is equivalent to the quantum description, in which temperature-independent fluctuations appear as a characteristic property of quantum systems. The study of this issue should serve us to establish contact with one of the distributions common to quantum statistical theory.

A. Including temperature-independent fluctuations

The distribution appropriate for considering all fluctuations cannot be of the form of Eq. (7a), as has been already established. Moreover in order to generalize Eq. (36) to include zero-point fluctuations we should look for a distribution $W_s(E)$ that maximizes the entropy and that yields

$$(\sigma_E^2)_s = U^2 \quad (63)$$

for every temperature, that is we require $(\overline{E^2})_s = 2U^2$ (the subscript s denotes averaging with respect to W_s to distinguish from the mean values calculated with W_g). The demand (63) is immediate by considering that the fluctuations come about from the interferences among a huge amount of independent modes, and therefore the central limit theorem applies.

According to the maximum entropy formalism,^[7] a distribution satisfying these constraints is given by

$$W_s(E) = \frac{1}{U} e^{-E/U}. \quad (64)$$

Obviously the selection $U = \beta^{-1}$ ($\mathcal{E}_0 = 0$) results in the usual canonical distribution Eq. (11) and leads to the classical expression, Eq. (36). But with the temperature-independent energy $\mathcal{E}_0 \neq 0$, U is given by Planck's spectrum and the resulting total fluctuations are (with U_T given by Eq. (40))

$$(\sigma_E^2)_s = U^2 = (U_T + \mathcal{E}_0)^2 = U_T^2 + 2\mathcal{E}_0 U_T + \mathcal{E}_0^2. \quad (65)$$

This shows that Eq. (36) can indeed be generalized to include the temperature-independent energy and fluctuations in the case $q \neq 0$. In the description afforded by W_s , at zero temperature the energy does not have a fixed value but is allowed instead to fluctuate with

variance \mathcal{E}_0^2 ; this term represents the temperature-independent fluctuations. For the thermal fluctuations we obtain from Eq. (65) (omitting the subscript s)

$$(\sigma_E^2)_T = \sigma_E^2 - \mathcal{E}_0^2 = U_T^2 + 2\mathcal{E}_0 U_T, \quad (66)$$

in agreement with Eq. (38), since both W_g and W_s yield the same *thermal* averages.

Let us now decompose the total energy into two fluctuating parts,

$$E = E_T + E_0. \quad (67)$$

where these terms stand for the (fluctuating) thermal and temperature-independent energies, respectively. The total fluctuations are then

$$\sigma_E^2 = \sigma_{E_T}^2 + \sigma_{E_0}^2 + 2\Gamma(E_T, E_0) = U_T^2 + 2\mathcal{E}_0 U_T + \mathcal{E}_0^2, \quad (68a)$$

where $\Gamma(E_T, E_0)$ stands for the covariance of its arguments,

$$\Gamma(E_T, E_0) \equiv \overline{E_T E_0} - \overline{E_T} \overline{E_0}. \quad (68b)$$

To write the second equality in (68a) we used Eq. (65). Using Eq. (66) for $\sigma_{E_T}^2$ and putting $\sigma_{E_0}^2 = \mathcal{E}_0^2$ leads to $\Gamma(E_T, E_0) = 0$, which shows that the fluctuations of E_T and E_0 are statistically independent, as was to be expected due to the independence of their sources.

The fact that σ_E^2 differs from zero at null temperature confirms that W_s is not limited to a thermodynamic description but affords a statistical one, which includes fluctuations beyond the thermal ones. This being the case, it is clear that the corresponding entropy S_s , defined using W_s in the relation (6), will not coincide with the thermal entropy in Eq. (3) derived from W_g , since the former should accomodate the new source of fluctuations. Such entropy is given by

$$S_s = -k \int W_s \ln W_s dE = k \ln U + k, \quad (69)$$

from which it follows that

$$\frac{\partial S_s}{\partial U} = \frac{k}{U}. \quad (70)$$

Comparison with the (thermal) entropy we have been using throughout the previous sections, which satisfies

$$\frac{\partial S}{\partial U} = \frac{1}{T}, \quad (71)$$

leads us to conclude that both entropies coincide only when $\mathcal{E}_0 = 0$ (and consequently $U = kT$). The existence of a fluctuating temperature-independent energy can be accommodated

for by introducing a "statistical" entropy S_s , as was done here, or equivalently a (quantum) redefinition of the temperature, $\beta \longrightarrow 1/U(\beta)$. A detailed discussion of these matters can be found in Ref. [17].

B. Quantum fluctuations and zero-point energy

We have seen that the statistical description afforded by the distribution W_s , Eq. (64), is linked to unfreezable zero-point fluctuations. On the other hand it is clear by now that the zero-point energy is crucial in going from a classical description to a quantum one. It therefore makes sense to investigate how these temperature-independent fluctuations manifest themselves in some statistical properties of the quantum systems. Here we limit our inquiry to a most immediate aspect.

Let us focus our attention on the quadratures q, p of the oscillator, related to its energy according to

$$E = (p^2 + m^2\omega^2 q^2)/2m. \quad (72)$$

To this end we should go over from the energy distribution given by Eq. (64) to a distribution $W(p, q)$ defined in the phase space (q, p) . We first note that $W(E)$ stands for a reduced probability density in the action-angle variables space (E, θ) (we omit the subscript s)

$$W(E) = \int_0^{2\pi} W(E, \theta) d\theta, \quad (73)$$

where

$$W(E, \theta) dE d\theta = W(p, q) dp dq. \quad (74)$$

Since $W(E, \theta)$ does not depend on θ for the equilibrium state, Eqs. (72) and (74) lead to^[18]

$$W(p, q) = \frac{\omega}{2\pi U} \exp\left(-\frac{p^2 + m^2\omega^2 q^2}{2mU}\right). \quad (75)$$

This distribution, which is known in quantum theory as the *Wigner function*,^[19] can be factorized as a product of two normal distributions,

$$W(p, q) = W_p(p)W_q(q) = \frac{1}{\sqrt{2\pi\sigma_p^2}} e^{-\frac{p^2}{2\sigma_p^2}} \times \frac{1}{\sqrt{2\pi\sigma_q^2}} e^{-\frac{q^2}{2\sigma_q^2}}, \quad (76)$$

where we have identified the variances $\sigma_p^2 = mU$ and $\sigma_q^2 = U/m\omega^2$. Thus we get that

$$\sigma_q^2 \sigma_p^2 = \frac{U^2}{\omega^2} = \frac{\mathcal{E}_0^2}{\omega^2} + \frac{\sigma_{E_T}^2}{\omega^2} \geq \frac{\mathcal{E}_0^2}{\omega^2} = \frac{\hbar^2}{4}, \quad (77)$$

where we have used Eq. (35) (with σ_E^2 written appropriately as $\sigma_{E_T}^2$) to write the second equality, and $\mathcal{E}_0 = \hbar\omega/2$ in the last one. We see that the magnitude of $\sigma_q^2\sigma_p^2$ is bounded from below because of the fluctuations of the zero-point energy (the minimum value $\hbar^2/4$ is reached when all thermal fluctuations have been suppressed). Eq. (77) allows to identify the origin of the Heisenberg inequalities with the presence of a *fluctuating* zero-point energy, and hence the descriptions afforded by thermal distributions such as W_g cannot account for their meaning, least of its origin. This result stresses again the fact that once a zero-point energy has been introduced into the theory, new distributions (specifically statistical rather than thermodynamic) are needed in order to include its fluctuations and to obtain the corresponding quantum statistical properties. It is also important to note that according to the present discussion, the Heisenberg inequalities should be understood as referring to ensemble averages, due to the statistical nature of Eq. (77) — or possibly to time-averaged quantities, if the system satisfies an ergodic principle.

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VII. APPENDIX A. ALTERNATE METHOD FOR DETERMINING THE PARITY OF $\sigma_E^2(U)$.

We have seen (Section III B) that the invariance of σ_E^2 under the inversion $E \rightarrow -E$ determines the parity of the function $\sigma_E^2(U)$, thus eliminating the parameter a_1 in Eq. (21). Here we present an alternate method to arrive at the same result, which allows to uncover the origin of this symmetry in both the classical and quantum cases.

We start from Eq. (21)

$$\sigma_E^2(U) = a_0 + a_1U + a_2U^2. \quad (78)$$

Together with Eq. (16) this gives

$$\frac{dU}{a_0 + a_1U + a_2U^2} = -d\beta. \quad (79)$$

By following a similar procedure to the one that lead from Eq. (24) to Eq. (26) we find that (26) generalizes to

$$U(\beta) = \begin{cases} \frac{1}{a_2\beta} - \frac{a_1}{2a_2}, & \text{for } q = 0; \\ \frac{\sqrt{q}}{2a_2} \coth \frac{\sqrt{q}}{2}\beta - \frac{a_1}{2a_2}, & \text{for } q > 0. \end{cases} \quad q \equiv a_1^2 - 4a_0a_2. \quad (80)$$

The roots of the equation $\sigma_E^2 = 0$ are now

$$U_{\pm} = \frac{-a_1}{2a_2} \pm \frac{\sqrt{q}}{2a_2}. \quad (81)$$

As we have seen \mathcal{E}_0 is one of the roots U_{\pm} and $a_2 > 0$, thus \mathcal{E}_0 corresponds to the largest of both roots (as before, the other one being unphysical), that is

$$\mathcal{E}_0 = \frac{-a_1}{2a_2} + \frac{\sqrt{q}}{2a_2}. \quad (82)$$

If the theory admits a null value for \mathcal{E}_0 the demand of finite relative dispersion at every temperature compels us to set a_0 and a_1 in (20) equal to 0. In this case $q = 0$, and from (80) we obtain $U = (a_2\beta)^{-1}$. As was done in Section IIIB comparison with the classical result leads to equipartition, Eq. (29).

If instead the theory allows for a zero-point energy $\mathcal{E}_0 \neq 0$, q can in principle acquire a value different from 0. Thus taking $q > 0$ gives using Eqs. (80) and (82)

$$\begin{aligned} U(\beta) &= \left(\mathcal{E}_0 + \frac{a_1}{2a_2} \right) \coth a_2 \left(\mathcal{E}_0 + \frac{a_1}{2a_2} \right) \beta - \frac{a_1}{2a_2} \\ &= \mathcal{E}_0 - \frac{\sqrt{q}}{2a_2} + \frac{\sqrt{q}}{2a_2} \coth \frac{\sqrt{q}}{2} \beta. \end{aligned} \quad (83)$$

Incidentally notice that this expression together with Eq. (16) gives the dispersion as a function of β ,

$$\sigma_E^2 = -U' = \frac{q}{4a_2} \left(\coth^2 \frac{\sqrt{q}}{2} \beta - 1 \right). \quad (84)$$

On the other hand, Wien's displacement law Eq.(2), namely

$$U(\omega, T) = \omega f(\omega/T), \quad (85)$$

is equivalent to the relation

$$\left(\frac{\partial U}{\partial \omega} \right)_T - \frac{U}{\omega} = -\frac{T}{\omega} \left(\frac{\partial U}{\partial T} \right)_{\omega}. \quad (86)$$

Taking into account that $\mathcal{E}_0 = \text{const} \times \omega$ and substituting (83) in the last equation we obtain

$$a_2 \mathcal{E}_0 \left(\mathcal{E}_0 + \frac{a_1}{2a_2} \right) \beta + \frac{a_1}{2a_2} \left[\frac{1}{2} \sinh 2a_2 \left(\mathcal{E}_0 + \frac{a_1}{2a_2} \right) \beta - \sinh^2 a_2 \left(\mathcal{E}_0 + \frac{a_1}{2a_2} \right) \beta \right]$$

$$= a_2(\mathcal{E}_0 + \frac{a_1}{2a_2})^2\beta. \quad (87)$$

Since we are assuming $q \neq 0$ (and thus $\mathcal{E}_0 + a_1/(2a_2) \neq 0$) it follows that a_1 must be 0 for this equation to be satisfied irrespective of the temperature. Further, Eq. (83) reduces to Eq. (30), and therefore, taking the high-temperature limit to set $a_2 = 1$ as before, to Planck's law.

It is interesting to observe that for $\mathcal{E}_0 > 0$, the even parity of the dispersion σ_E^2 as a function of U is a direct consequence of Wien's law (which entails $\mathcal{E}_0 \propto \omega$). In the classical case ($\mathcal{E}_0 = 0$) it was the demand that the relative dispersion remains finite at $T = 0$ which lead us to a similar conclusion about the parity of σ_E^2 .

VIII. APPENDIX B. THE VALUE OF $\overline{\ln g(E)}$.

We have seen that the mean value of a general function $f(E)$ calculated with W_g is

$$\overline{f(E)} = \frac{1}{Z_g} \sum_m f(E_m) e^{-\beta E_m} = \sum_m f(E_m) w_m. \quad (88)$$

Let us apply this to the function g given by Eq. (59),

$$f(E) = \ln g(E) = \ln \sum_{n=0}^{\infty} 2\mathcal{E}_0 \delta(E - E_n), \quad (89)$$

whence

$$\overline{\ln g(E)} = \sum_m \ln \left[\sum_{n=0}^{\infty} 2\mathcal{E}_0 \delta(E_m - E_n) \right] w_m. \quad (90)$$

We write the single contribution for $n = m$ as $1/\varepsilon$ with $\varepsilon \rightarrow 0$. Since ε is a numeric constant independent of m , it can be taken out of the sum, which results in

$$\overline{\ln g(E)} = \ln \frac{1}{\varepsilon} \sum_m w_m = \ln \frac{1}{\varepsilon}. \quad (91)$$

We verify that $\overline{\ln g(E)}$ is a numeric constant independent of β , as asserted in the main text.

That $\overline{\ln g(E)}$ should be a constant follows also from the observation that according to the formalism of maximum entropy^[7] the distribution

$$W_g = \frac{1}{Z} e^{-\beta E + \ln g(E)} \quad (92)$$

corresponds to a simultaneous stationary value of the entropy and of $\ln g(E)$.

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